Comments to editor

Thankyou for considering our paper for AMT. We added a lot of content to the paper and much of it answers multiple reviewer comments, so it seemed impractical to quote everything we did in this document. We've therefore just restructured the public review responses: discussion is in red text and description of changes is in magenta.

Our main changes are to include the details requested by reviewer 1 along with additional analysis which we believe to be a reasonable, but strict, test of how AOD spatial variability may affect our results. We show that the effect of AOD is generally small, and point out that in practice we can likely identify cases in which it is not small.

Reviewer 2 recommended rejection in the manuscript's original form, we have now addressed their concerns. This involved adding approximately 2.5 pages of detail, two figures and several equations. In summary: we had actually largely followed the methodology they suggested as the standard way of doing things, as part of our published companion paper. However, we had not explained this (or some other details) well, and so we have now clarified everything they mention.

One concern of theirs that we didn't address was that we did not perform full 3-D radiative transfer for all of the LES outputs. Our approach is nevertheless standard and we argue that it is clearly publishable – we do not have the capacity to do full 3-D simulations and are not aware of any cases where those have been done for the data volumes we require, specifically with very high spectral resolution. We do not believe our paper should be rejected for its use of plane-parallel radiative transfer, which is a common tool in many recently published papers.

Reviewer 1 response in on p2—6, reviewer 2 response on p7—11.

Reviewer 1

This well written manuscript deals with future spaceborne imaging spectrometers expected to measure water vapour columns with horizontal resolutions of < 100 m. The authors simulate biases in water vapor scaling statistics that will occur at high solar zenith angles due to a solar light path traversing neighboring pixels. To reduce the biases, the authors propose a sampling strategy perpendicular to the solar azimuth angle. This is evident, and the described bias reduction is what one would expect. The merit of this study, which fits very well to AMT, is a quantification of the expected biases in water vapor scaling statistics. The study still lacks details on assumed measurement uncertainties, see specific comments.

Thanks for taking the time to read and think about our paper. We have added the requested details on uncertainty and additional tests on the effect of AOD.

The main text includes new Figure 2(e) and Figure 5(e) panels showing the AOD results, plus text discussing those, and in the discussion & conclusions. We believe these additions are demonstrate our AOD-relevant conclusions without unnecessarily lengthening the paper. We include extra details in this review response to help the reviewer(s) judge our methodology.

A lot of text and 2 figures were added to respond to reviewer 2 – we kept your comments in mind and responded to them where possible in this added content.

Specific Comments:

1. Spatially nonuniform aerosol distributions (as stated in the abstract) are in my opinion not enough addressed. They probably pose the highest challenges to spectroscopy. On the other hand, they may be difficult to assess, and the resulting biases difficult to quantify. It would nevertheless be of high merit to include them in your model framework and to show some related simulation results in section 2.

DISCUSSION

Tucked away in Supplementary Figure 7 of our last paper we showed that $TCWV_{ret}$ isn't that sensitive to AOD, and our emulators were developed with randomised AOD. We anticipated that with typically small(ish) horizontal gradients in AOD over <1 km there would be minor effects on our results from AOD.

However, this paper really should demonstrate this rather than state it, so we added AOD results in the new Figure 2 and added an AOD-results panel to Figure 5.

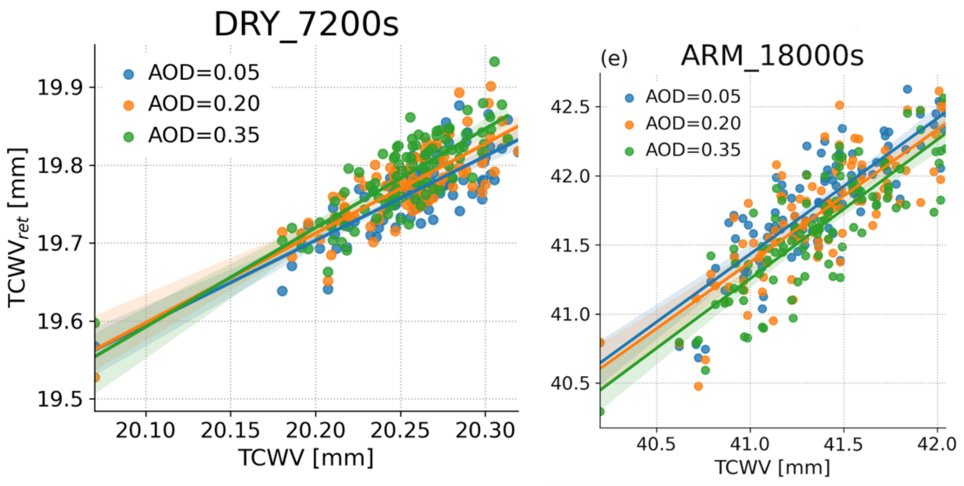
Our approach was to generate a "very very bad case" with large AOD gradients of order 0.3 km^{-1}, and show that it has a small effect on estimated ζ_2. The paper shows the ARM_18000s example, it represents the 22 out of 23 cases where the effect on exponents is small. We expand on this here in case the reviewers are interested. If you only care about further summary of main-text changes, see bolded paragraph at the end.

Additional detail for reviewers

The original emulators were fit to forward & inverse simulations with randomised true AOD. We re-ran ARM_18000s and DRY_7200s forward and inverse simulations with profiles where AOD is fixed at 0.05, 0.20 or 0.35 and generated new emulators. We used these emulators *only* for the specific AOD sensitivity tests.

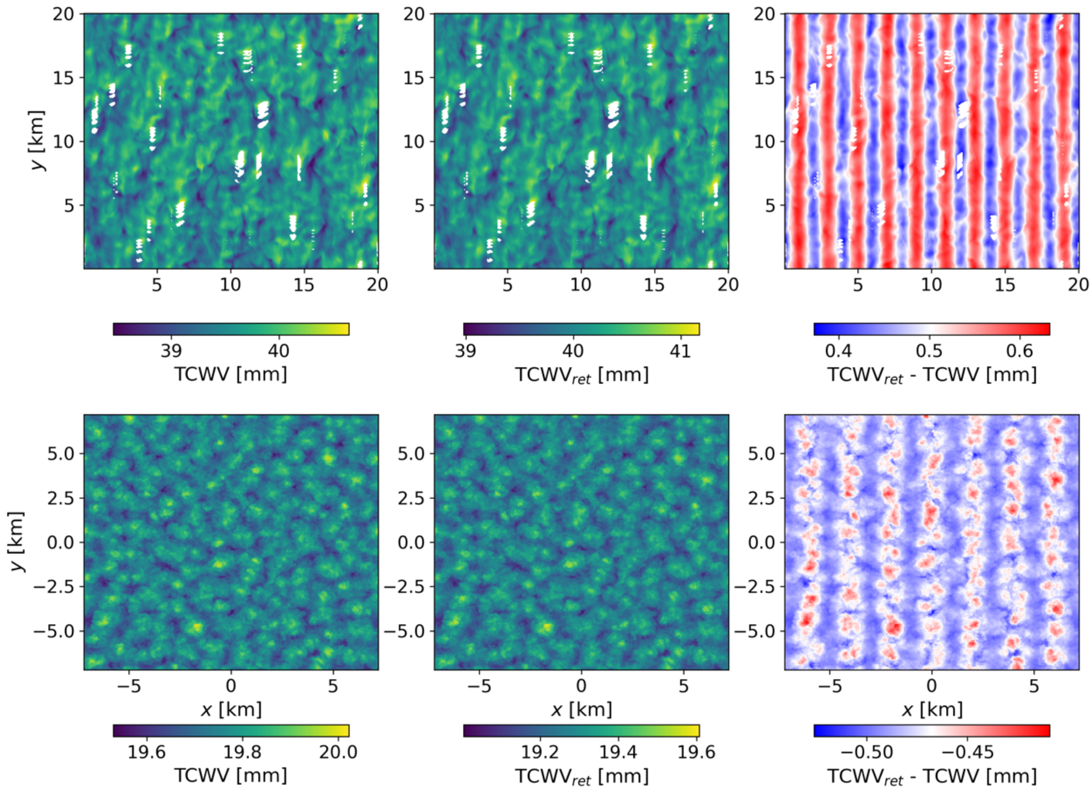
ARM_18000s saw a shifting mean bias of ~0.3 % in $TCWV_{ret}$ when AOD changes from 0.05—0.35. The changes are proportionally smaller for DRY_7200s but include changes in gradient. For our first test we modified our emulators to make the gradient and intercept into functions of AOD and fit them:

$$TCWV_{ret} = a_1(AOD)TCWV_{eff} + a_2(AOD) + \epsilon$$



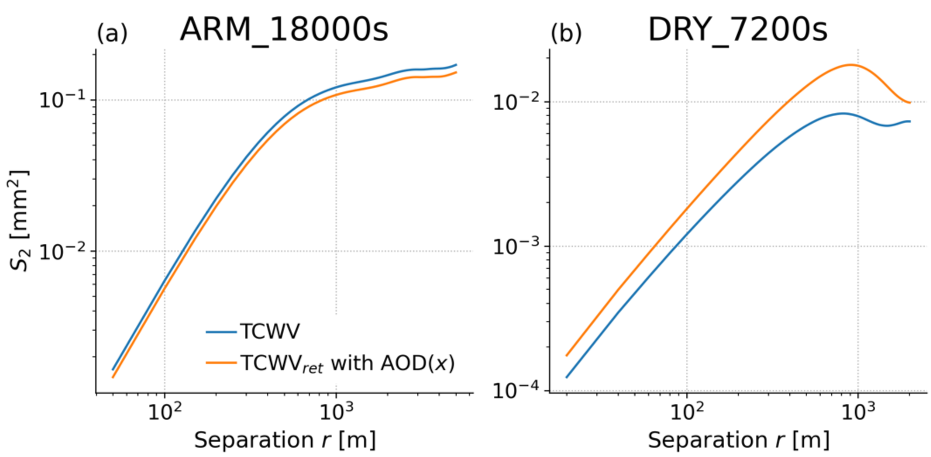
The panels above show the fits that provide sets of a_1 and a_2 values given AOD in [0.05, 0.20, 0.35]. For any AOD we simply linearly interpolate between those to provide our AOD-dependent emulator. The next issue was to decide what sort of spatial variability in AOD to test.

We decided on a rather extreme case: changes from 0.05—0.35 every 1 km, represented by a horizontally-varying sinusoid with period 2 km in either the *x* or *y* direction. Below is true TCVW, emulated TCWV and the difference between them for DRY_7200s and ARM_18000s at SZA=0°. The horizontal waviness from the spatial AOD structure is obvious in (c,f). We did not add random error (ϵ) here, but the paper shows that we can identify and remove its effect on S_2. (ARM masked values are those that are cloudy or shaded at any of our selected SZAs).



Next, we address how S_2 and ζ_2 respond, firstly in just these two snapshots. The figures below show they are offset: this is primarily because of a_1 – it scales S_2 as shown and discussed in main paper Figure 5(c). Note that panel (a) below differs from the new Figure 5(e) for reasons discussed below.

This DRY case is the outlier value with the lowest ζ_2 of all snapshots, and it's clearly due to the "dip" near ~1 km separation suppressing the gradient. As discussed in the paper, we do not investigate the detailed dynamics of the LES cases here but are only interested in how well we can retrieve the property. In the ARM case the change in ζ_2 is negligible (0.63 vs 0.63), but in DRY_7200s changes greatly from ~0.2 to ~0.4.

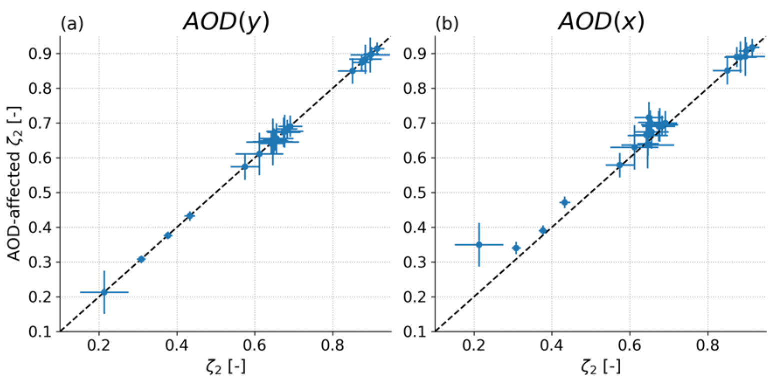


The DRY_7200s difference occurs because the true S2 structure shows a decrease in variance near ~1 km while our AOD-induced variability has a maximum effect at 1 km separation. We wanted to test all snapshots but didn't have time to process the forward and inverse simulations needed to generate individual emulators, so we used another approximation. In percentage terms, the ARM_18000s case shows the largest effect: a 0.1 % change in $TCWV_{ret}$ per 0.1 change in AOD, so we used that as the basis of our next test.

We added a simple treatment of aerosol to all emulated snapshots: a sinusoidal variation in x or y of $TCWV_{ret}$ with an amplitude of ±0.15 % of the field mean and a wavelength of 2 km. This is just like the test above, except there is no change in a_1. For Figure 5(e) the test uses $a_1 = 1$, so the S_2 lines lie atop each other rather than have the offset seen in the above figure.

This results in a change of 0.3 % in $TCWV_{ret}$ every 1 km to represent a change of ~0.3 in AOD over that distance. The next figure shows how the difference is negligible when calculated perpendicular to the aerosol variation (see panel a) but when calculated parallel to the aerosol variation (panel b) there are changes. The direction dependence is rather like our sensitivity to solar azimuth. From this figure the DRY_7200s case is the outlier of the set: changes in non-DRY snapshots are always <4 % in magnitude, for the DRY snapshots except DRY_7200s it is ~10 %.

One nice thing about ISOFIT is that we would have $TCWV_{ret}$ and retrieved AOD fields, so we could "back calculate" the likely effects of AOD on retrieved ζ_2 and flag cases where it might be important. We have referred to this briefly in the new text.



CHANGES TO MANUSCRIPT

In summary: we hope this review response persuades the reviewer that we did our due diligence for AOD. In the main paper we have added the following:

i. Figure panel 2e showing how $TCWV_{ret}(TCWV)$ changes as a function of AOD in ARM_18000s
ii. Figure panel 5e showing how S_2 changes with a strong spatial variation in AOD in ARM_18000s
iii. Text summarising changes in ζ_2 are generally small even with relatively large AOD gradients, and noting that while it has a large effect in one snapshot, we could use the ISOFIT retrieved fields to flag cases where this is likely in practice. AOD-relevant text is in Sections 2.2, 3.2 and 4.

We think these changes strike the balance between being sufficient and brief.

2. In section 2.2 you define parameters related to assumed measurement uncertainties and biases. Since they are used throughout the study, it would be good to describe them better here, perhaps including a figure which illustrates sensitivity (a1) and bias (a2). In addition, you should be more specific concerning the impact of aerosol layers (comment 1), and concerning probable error correlations between (for example) surface albedo and aerosol concentration variations. Finally, can you assess the impact of simulation idealizations and simplifications which you have likely undertaken?

CHANGES TO MANUSCRIPT

Our completely restructured Section 2 aims to address these comments. The new Figure 2 shows how changes in individual properties (SZA, surface, AOD) change the response. Our new text emphasises that we propose retrieving only over mixed-vegetation or mixed urban-mineral surfaces, which have similar characteristics. We would also have near-constant SZA in our samples. Since surface type and SZA effects will be near constant if our method is followed, we do not think it is important to include covariance with AOD.

Covariance between the LES-simulated q(z)/T(z) and aerosol is implicitly included in our development of the emulators, so we believe we have now displayed the things that matter for our application.

Technical Comments:

p.5 line 3: "with CWP calculated in the same manner as the TCWV": also pressure-weighted? Likely not.

DISCUSSION

Actually yes, given the units we had. This text has now been deleted though.

CHANGES TO MANUSCRIPT

Section 1 new text explains our different path definitions for water vapour and Section 2.2.2 describes the calculation. In hindsight the "pressure weighting" is redundant information – there is only one way to convert our path-traced values into units of mm so we removed that term.

p.7 line 6: "random errors that we estimate": please give examples (numbers) for these errors, in % of the TCWV.

CHANGES TO MANUSCRIPT

Added. We slightly rephrased and added: "(0.6 % of TCWV in this case)". This was the σ_{ε} discussed in the emulator equation, and the OSSE range was 0.5—0.7 % of mean TCWV depending on the LES case (values in mm are in Richardson et al., 2021, Table 2).

Citation: https://doi.org/10.5194/amt-2021-163-RC1

Reviewer 2

This manuscript documents an OSSE-type (Observation System Simulation Experiment) study of how the high-spatial resolution spectroscopy observation of total column water vapor from satellite observations should be sampled to understand the horizontal variability and structure of water vapor in the planetary boundary layer (PBL).

Topic of this study is important and suitable for the AMT. However, the manuscript suffers from several major issues and significant flaws as pointed out below. Its methodology (i.e., using a simple emulator instead of full simulator) is not justified and has serious potential problems. No causes and underlying physics are provided for the "solar-smearing bias", which is a key finding of this study. Even though the methodology is problematic, and the results are not explained, the authors still try to propose a universal "new sampling strategy" to the current and future high-resolution spectroscopy sensors. This is overreaching the say the least and could be misleading.

Based on these considerations, I strongly recommend rejection of this manuscript. It this study were published, the "emulator method", the "solar-smearing bias", and "new sampling strategy" could be cited again and again as if they were correct. But they are not, at least not justified by this study.

We thank the reviewer for their rigorous approach, which made it obvious that we had not been explicit enough about important details. Some other readers could clearly be confused by our original submission, so we have added two new figures and text to hopefully avoid this confusion. We believe that all reviewer concerns are now addressed.

Below we reference page and line numbers, which refer to those in the *red lined/track changes* version of the manuscript.

Major problems:

- The first major problem of the manuscript is the lack of important details on the methodology and the discussions are often too short and unsatisfying.
    - Although the concept of "total column water vapour" (TCWV) appears to be simple, the retrieval process can be quite complicated and involves many technical details, especially at high-spatial resolution. For example, when water vapor has both strong horizontal variation and vertical gradient, the solar-viewing geometry will become important because the path-integrated water vapor can be significantly different from the TCWV, depending on how instrument geolocation/collocation is done. In such situation, observations from different angles need to be de-convoluted to re-construct the horizontal and vertical structure of water vapor. The manuscript briefly mentioned this issue in section 2.2 and 3.1 but the discussion is far from clear or satisfying. For example, it is mentioned "TCWVret from input TCWV, which is in fact the integrated water path along the solar path". But how is the "path-integrated water path" converted back to the TCMV (only times a cosine factor?)? Is the definition of TCWV dependent on solar and/or viewing angle? Although Figure 2 provides some information on the vertical variation of water vapor of

the cases used in this study, the corresponding discussion in Section 3.1 is so brief (only one sentence) and obscured that it only raises more questions than answers. In particular, it is hard to tell how the author could "confirm that our derived values are indeed representative of bulk PBL statistics" from the figure, when there seems to be significant vertical variation of epsilon in the PBL.

DISCUSSION

Here is where we realised we explained some of our most important method details very poorly.

Our "solar smearing" refers to how the non-vertical solar path through the atmosphere, which cuts through a complicated 3-D field, "smears" the apparent 2-D retrieved TCWV maps. This is explained in new content as detailed below.

All current imaging spectrometer retrievals of atmospheric water vapor ignore this effect when reporting the TCWV; in other words, they do not perform the tomographic reconstruction that the reviewer rightly calls for. To our knowledge, our study is the first that attempts to account for these effects with this class of instruments.

Please see response to next comment for details on how the path-dependence is included in the radiative transfer calculations behind our emulator, and how it is also accounted for in the emulator inputs.

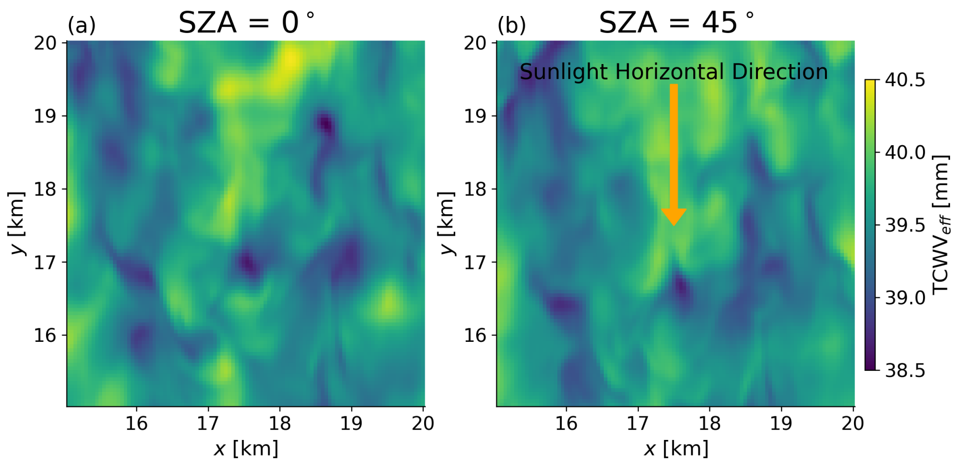
CHANGES TO MANUSCRIPT

We have now added detail in Section 1 on p3L30 onwards and Figure 1. We added equations and description that relate path integrated water vapour (PIWV), real TCWV, and the reported "TCWV" retrieved by VSWIR instrument. We use TCWV terminology for consistency with other VSWIR work, citing 6 papers that call their retrievals "TCWV", although we use subscripts to differentiate properties. In particular, we refer to "effective" TCWV:

$$TCWV_{eff} = \frac{PIWV}{\frac{1}{\mu} + \frac{1}{\mu_0}}$$

Which is the TCWV that would provide the same PIWV given the solar/view geometry. The PIWV is determined from tracing the solar ray through the atmosphere, and our retrieved $TCWV_{ret}$ are estimates of this $TCWV_{eff}$.

Figure 1 compares TCWV and PIWV when SZA=45° in a small part of an LES snapshot domain. An arrow indicates the horizontal component of the solar path; it is visibly obvious that the IWV field is like the TCWV field but "smeared" or "smoothed" in the horizontal. This is simply the result of the solar downward path being diagonal, rather than vertical.



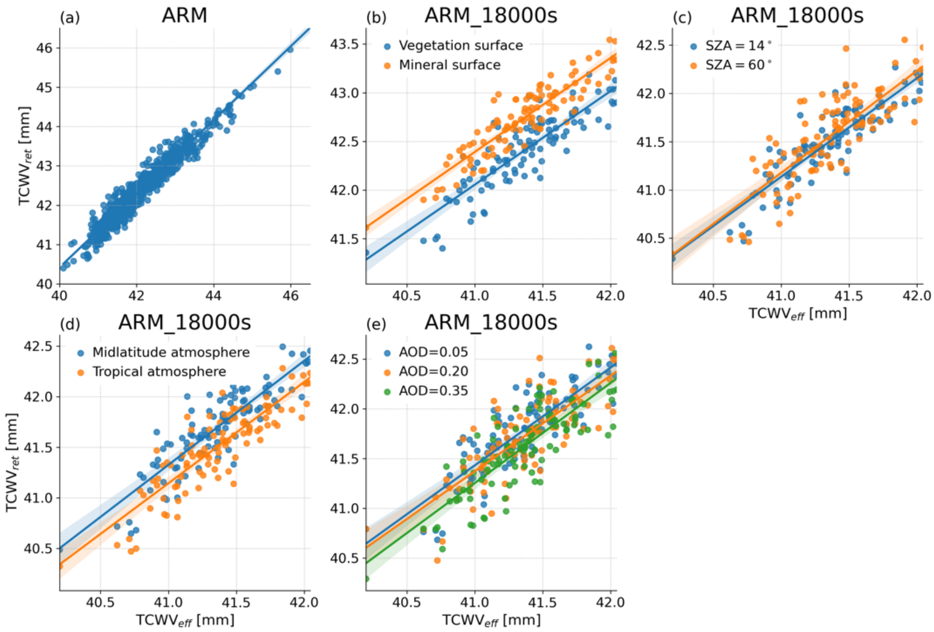
We also changed "confirm that our derived values are indeed representative of bulk PBL statistics" to "…are indeed representative of ζ_2 derived from $PCWV_{PBL}$" since we retrieve the value derived from bulk PBL water vapour, not the average of exponents calculated at higher vertical resolution.

- Some other technical details are also missing. For example, how cloud mask is applied? Is it dependent on the sun-viewing geometry? If cloud mask is independent of sun-viewing geometry then there is apparently an inconsistency between the use of path-integrated TCWV and use of path independent cloud mask. Is the 3-D radiative transfer considered in the simulation or emulation? Previous studies have noted the "halo effects" of cloud in the so-called twilight zone. How are these 3-D effects of cloud treated in the study? Are they simply ignored (i.e., using 1-D RT model), or removed by cloud masking (then how?) or considered in the simulation?

CHANGES TO MANUSCRIPT

We have split Section 2.2 into two sections. Subsection 2.2.1 is almost entirely new text which describes the OSSE approach: we used 1D RT (MODTRAN) and an optimal estimation inverse method (ISOFIT) to derive the emulator, for which we found Eq. (4) (now Eq. 8) was an adequate representation.

Subsection 2.2.1 also refers to a new Figure 2, which demonstrates the linear relationship we assert for the emulator, and shows how the parameters may change with surface, SZA, retrieval-assumed $q(z)/T(z)$ and AOD.



Subsection 2.2.2 now expands on the ray tracing we used to generate and explicitly states that we use the $TCWV_{eff}$ derived from ray-traced PIWV through the 3-D LES field as input to our emulator. We hope that, in combination with the additional detail in Subsection 2.2.1, this is now clearer. Given this context we believe readers can now understand how our cloud/shadow mask is generated in a completely analogous way: "The same ray-traced calculation is repeated with cloud water q_c to obtain cloud water path (CWP). Footprints are then flagged as cloudy or shaded when CWP>1×10^{-3} mm…".

We agree with the reviewer that 3-D radiative effects could be very important. These would be implicitly addressed by our suggested airborne experiment but we were remiss in not specifically mentioning it. As noted in the new 2.2.1 text, we did not have the computational resources for 3-D RT across all of our desired cases, especially given our very high spectral resolution requirements. Section 4 now mentions that 3-D RT forward modelling is a good way to improve this: we reference papers behind SHDOM and MYSTIC here.

- The use of a very simple retrieval emulator is not justified and raises many questions.
  - OSSE type of studies often use a "retrieval simulator" consisting of a "forward" RT simulator and an "inverse" retrieval simulator. The simulator should be as "realistic" as possible in comparison with the real retrieval to faithfully capture the influences of various factors on the retrieval. In contrast, this study only uses a seemingly naïve retrieval "emulator" (i.e., equation 4) and the only reason to justify this is "due to computational constraints". This "emulator" skips both the RT simulation process and the retrieval simulation step, and directly connects the retrieval to the input fields in a very simple way (linear). There is no discussion on the accuracy of this emulator in comparison with the "full OSSE simulator" if there is one. As a result, it is unclear if the artifacts in the "retrieval" is meaningful or simply due to the inadequacy of the emulator. It is also hard to imagine what kind of "computational constraints" the authors are referring to. This is a case study based on a handful of LES scenes. Many previous studies have performed full RT simulations, even 3-D

RT simulations, based on LES scenes. How and why is the RT or retrieval simulation in this study so computationally expensive?

DISCUSSION

Please see responses above. The reviewer describes what we believe to be the "correct" way, which is indeed what we did in Richardson et al. (2021). The new 2.2.1 text describes the previous OSSE from which Eq. 8 (originally Eq. 4) is derived, and the new Figure 2 (above) shows some evidence that should persuade readers to provisionally accept the linearity between $TCWV_{eff}$ and $TCWV_{ret}$. More details are in our previous publication.

- The solar-geometry dependent retrieval bias in section 3.3 is interesting. However, I tried hard to find some explanation of the causes and underlying physics but didn't find any. There is neither any reference to previous studies or discussion on whether this phenomenon had been discovered before or completely new. **The authors didn't even bother explaining why this bias is called "solar-smearing" effect.** The word "smear" only occurred twice in the manuscript, one in the title and the other in the conclusion.

DISCUSSION

Again our failure to sufficiently link back to Richardson et al. (2021) caused confusion.

CHANGES TO MANUSCRIPT

The new text in Section 1 mentioned above describes the physical principle, namely the solar path through a 3-D field and explains why we pick the term:

"The **Error! Reference source not found.**(a) to **Error! Reference source not found.**(b) differences show a smoothing or smearing in the *y* direction, so we refer to these solar-geometry induced changes as the "solar smearing" effect." (figure 1 is the first shown in this review response)

- Event though the "solar-smearing" effect is completely unexplained (and is based on highly questionable methodology), the authors still recommended the "new sampling strategy" to many current and future sensors. This totally unacceptable to me.

DISCUSSION

The reviewer was right to be cautious given the lack of clarity in our original submission, but we are convinced that the concerns you rightly raised are now addressed. After all, with the exception of 3-D radiative transfer, we actually performed the calculations in ways that you proposed (an OSSE with forward an inverse models) and directly accounted for issues you raised (the complex 3-D structure of the water vapour field).

CHANGES TO MANUSCRIPT

Regarding 3-D radiative transfer, this was a limitation of our available tools and computational resources but it is a very good suggestion which we now mention in the discussion & conclusions.